

FIG. 1A

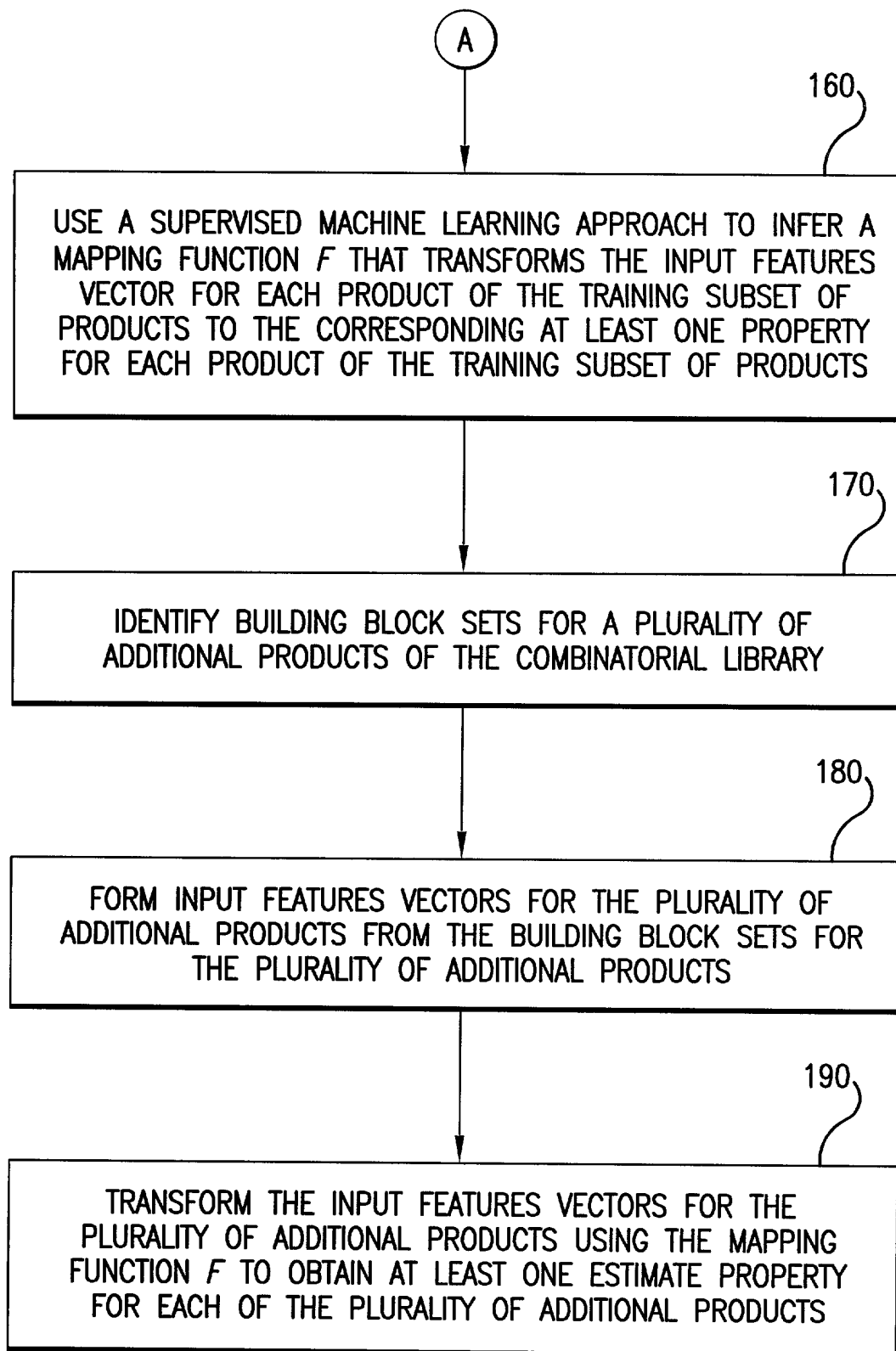


FIG. 1B

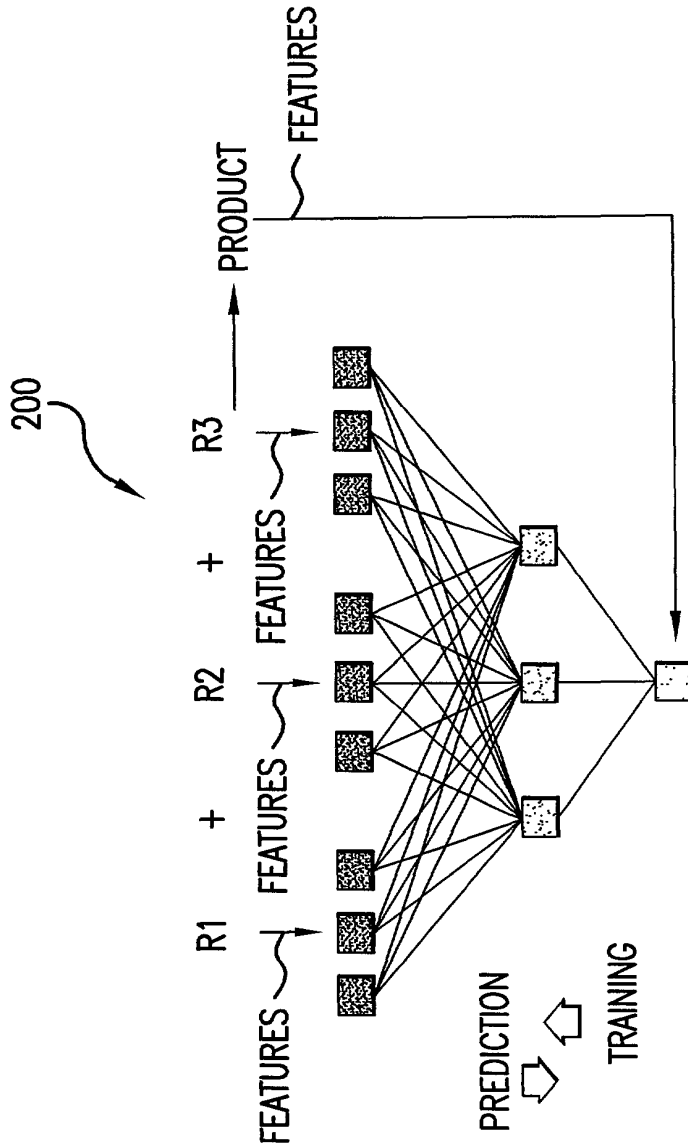


FIG.2

Appl. No. 09/934,084; Group Art Unit: 2857
 Dkt. No. 1503.1070003; Batch No.: N/A
 Inventor(s): Lobanov et al.; Tel: 202/371-2600
 Title: Method, System, and Computer Program Product for
 Determining Properties of Combinatorial Library Products...

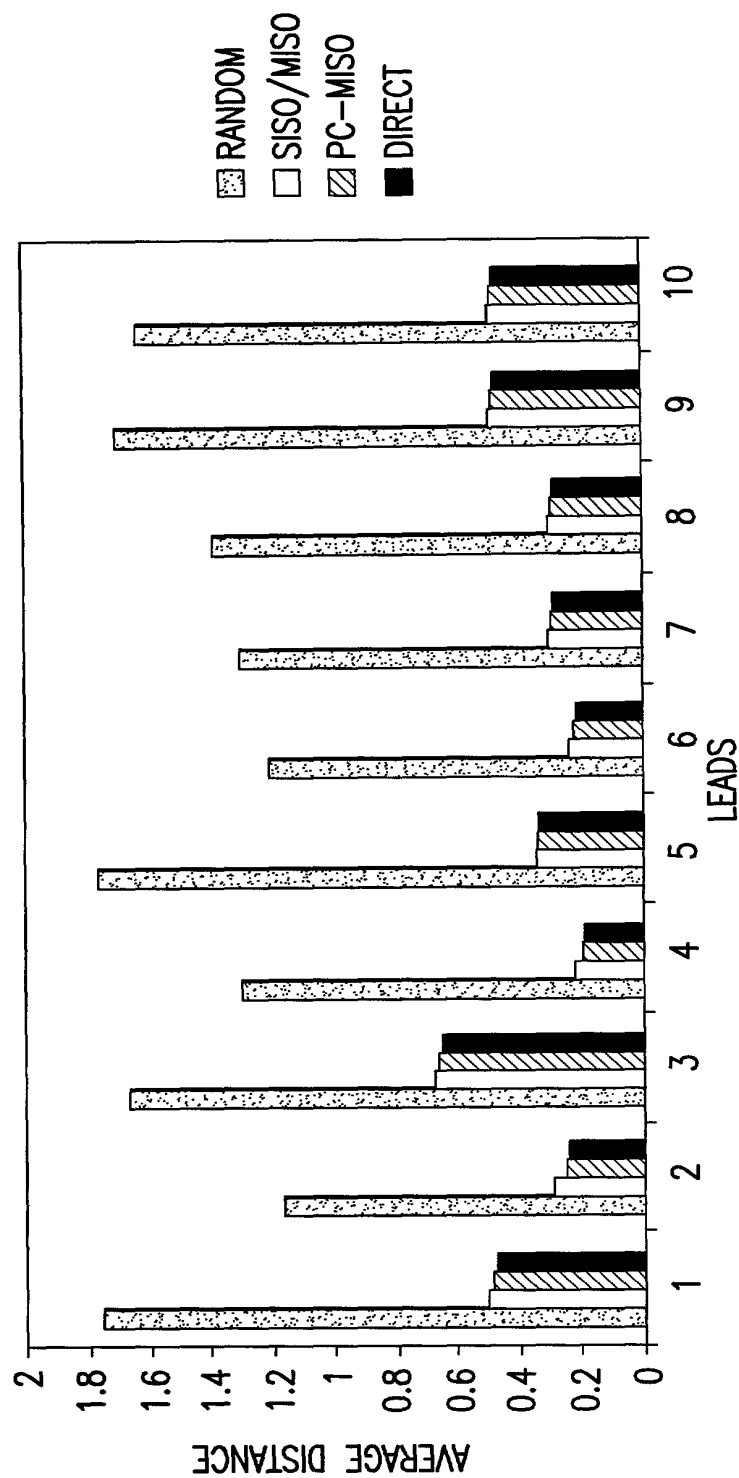


FIG. 3

Appl. No. 09/934,084; Group Art Unit: 2857
 Dkt. No. 1503.1070003; Batch No.: N/A
 Inventor(s): Lobanov et al.; Tel: 202/371-2600
 Title: Method, System, and Computer Program Product for
 Determining Properties of Combinatorial Library Products...

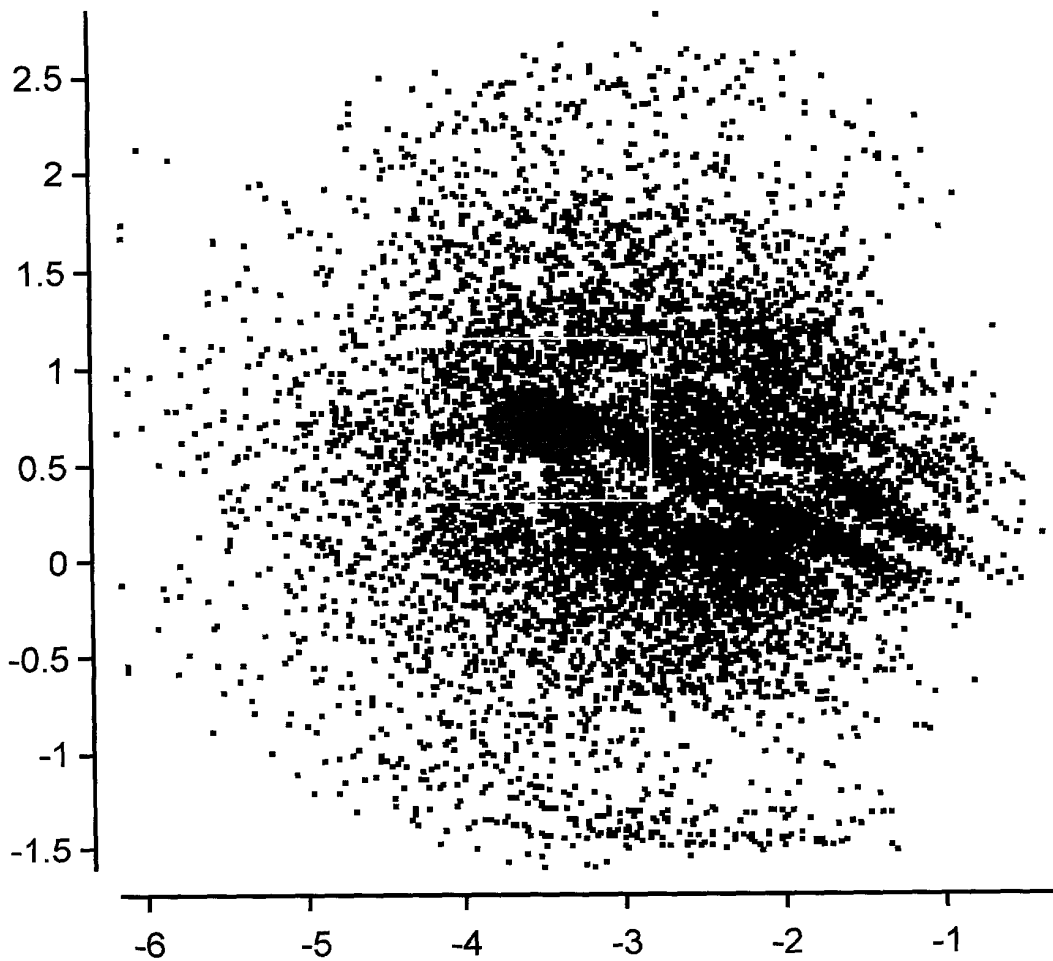


FIG.4A

Appl. No. 09/934,084; Group Art Unit: 2857
 Dkt. No. 1503.1070003; Batch No.: N/A
 Inventor(s): Lobanov et al.; Tel: 202/371-2600
 Title: Method, System, and Computer Program Product for
 Determining Properties of Combinatorial Library Products...

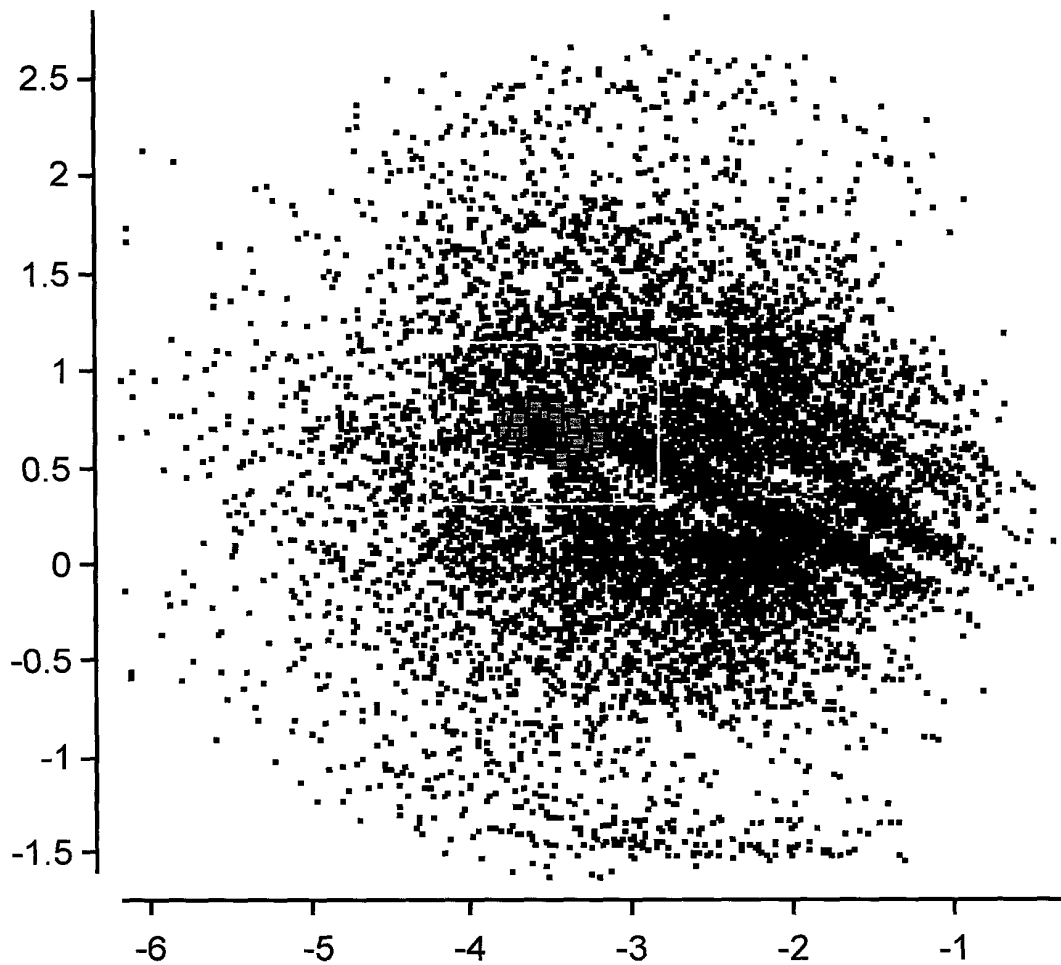


FIG.4B

Appl. No. 09/934,084; Group Art Unit: 2857
 Dkt. No. 1503.1070003; Batch No.: N/A
 Inventor(s): Lobanov et al.; Tel: 202/371-2600
 Title: Method, System, and Computer Program Product for
 Determining Properties of Combinatorial Library Products...

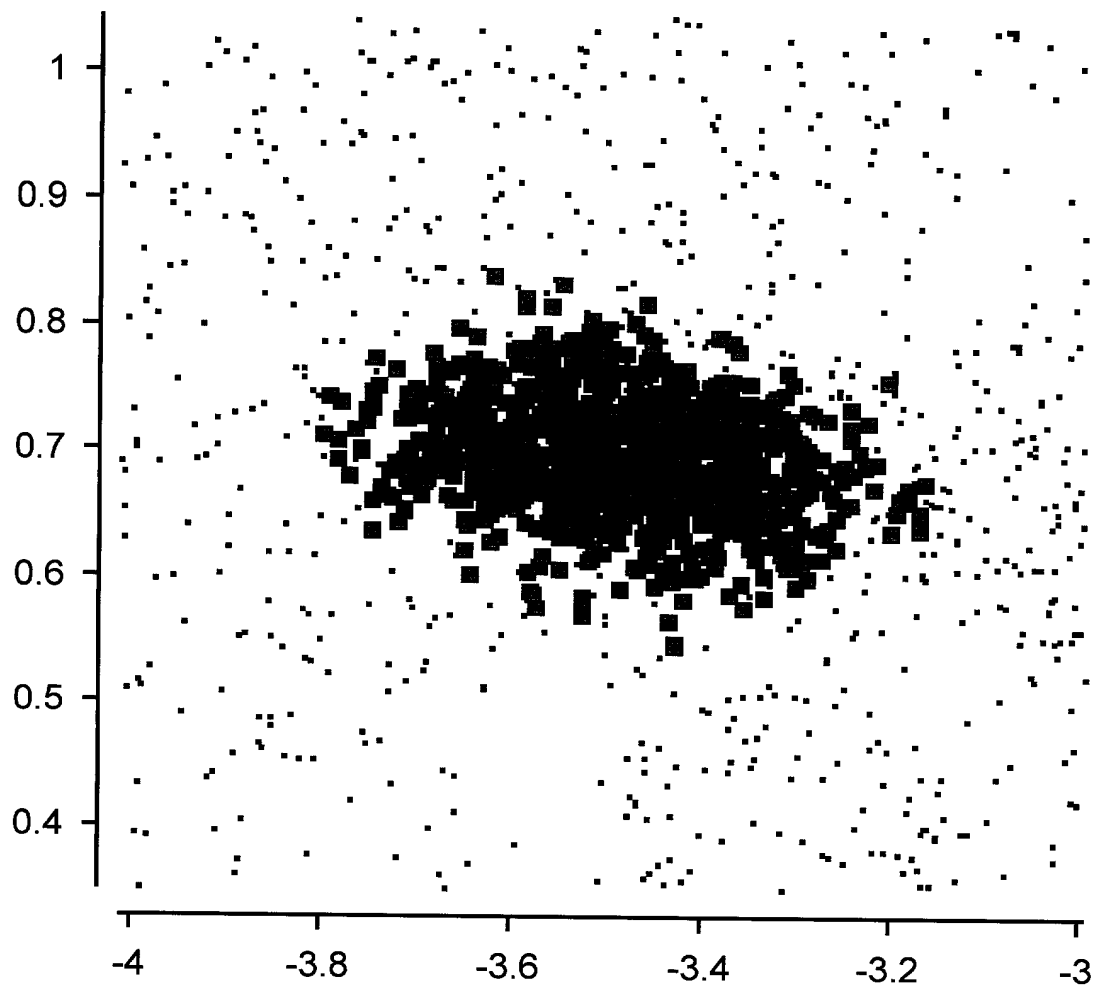


FIG.4C

Appl. No. 09/934,084; Group Art Unit: 2857

Dkt. No. 1503.1070003; Batch No.: N/A

Inventor(s): Lobanov et al.; Tel: 202/371-2600

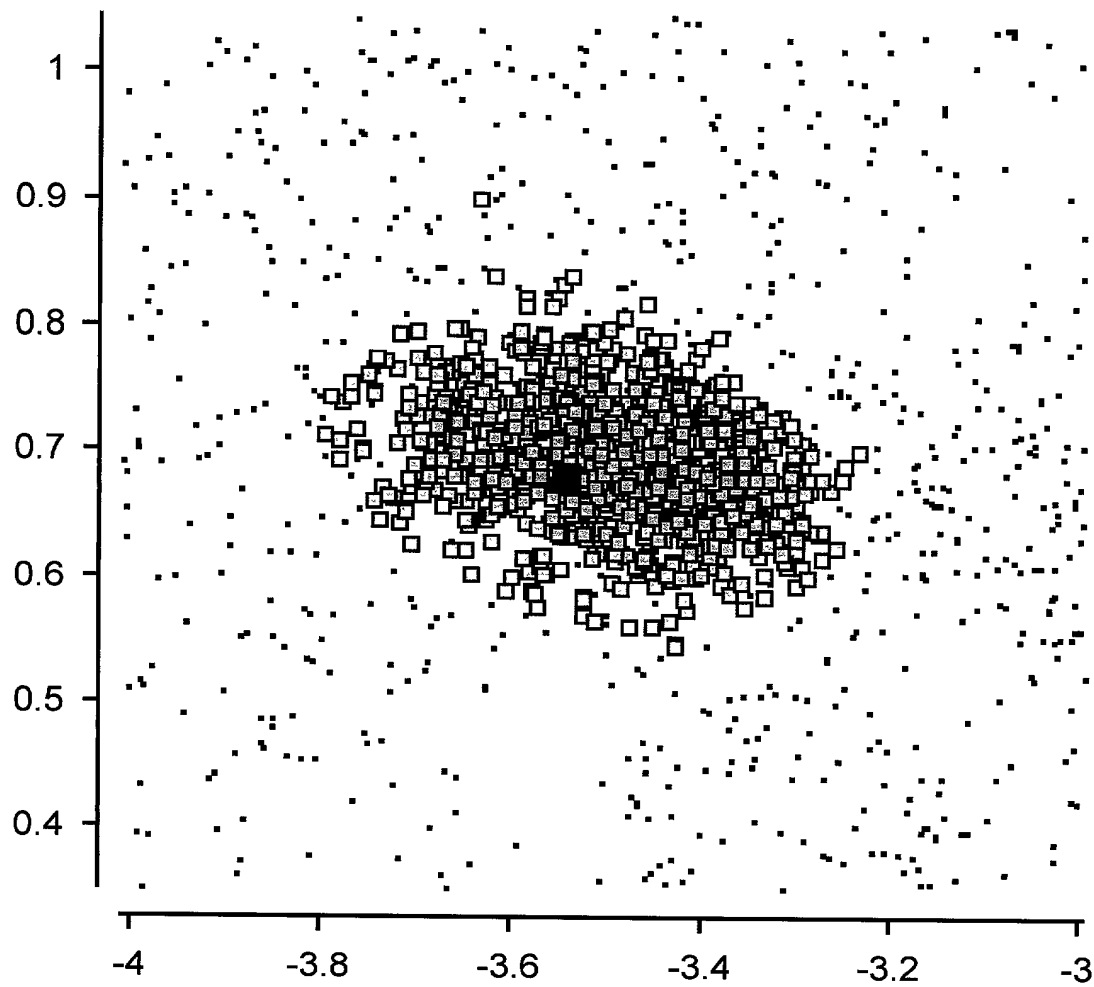
Title: Method, System, and Computer Program Product for
Determining Properties of Combinatorial Library Products...

FIG.4D

Appl. No. 09/934,084; Group Art Unit: 2857

Dkt. No. 1503.1070003; Batch No.: N/A

Inventor(s): Lobanov et al.; Tel: 202/371-2600

Title: Method, System, and Computer Program Product for
Determining Properties of Combinatorial Library Products...

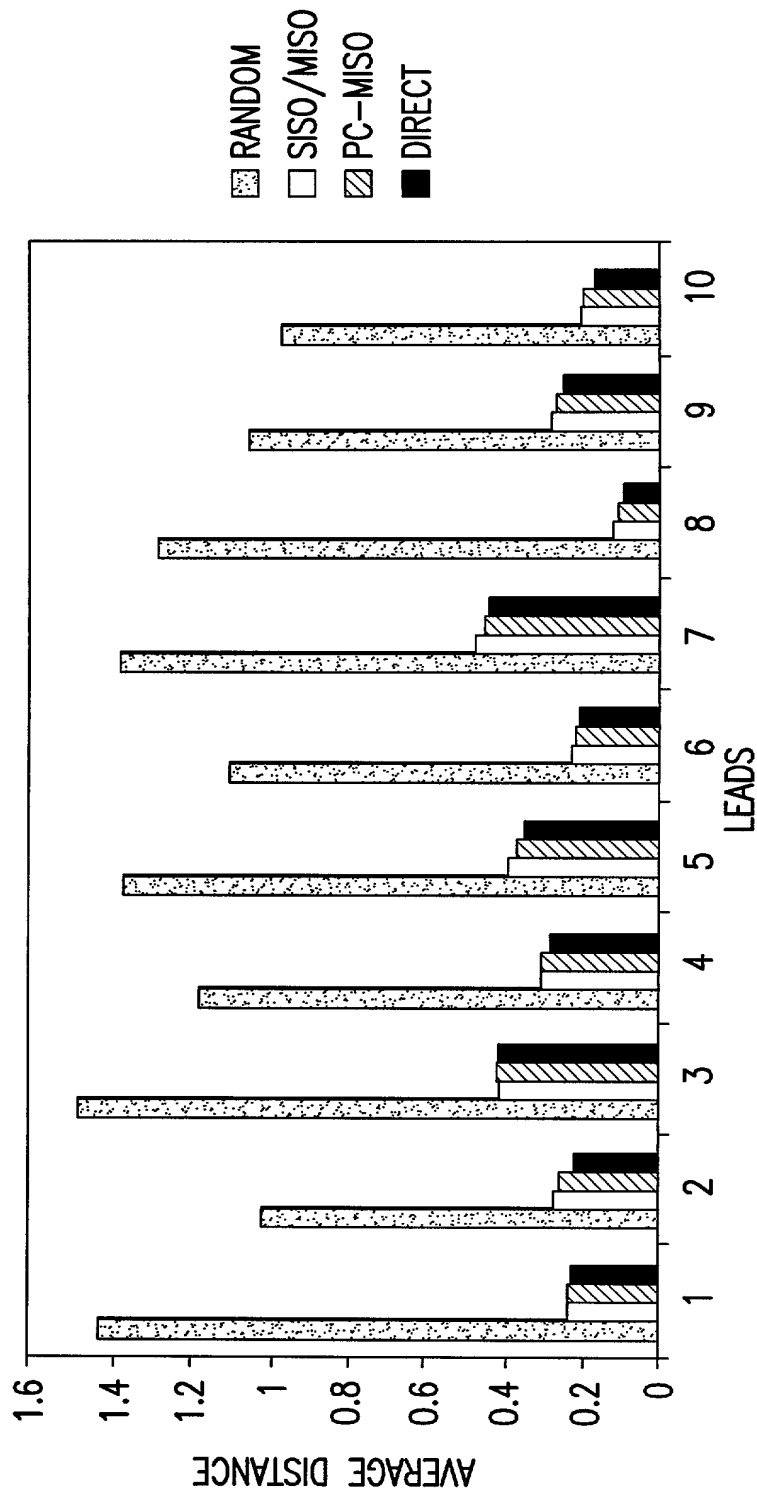


FIG.5

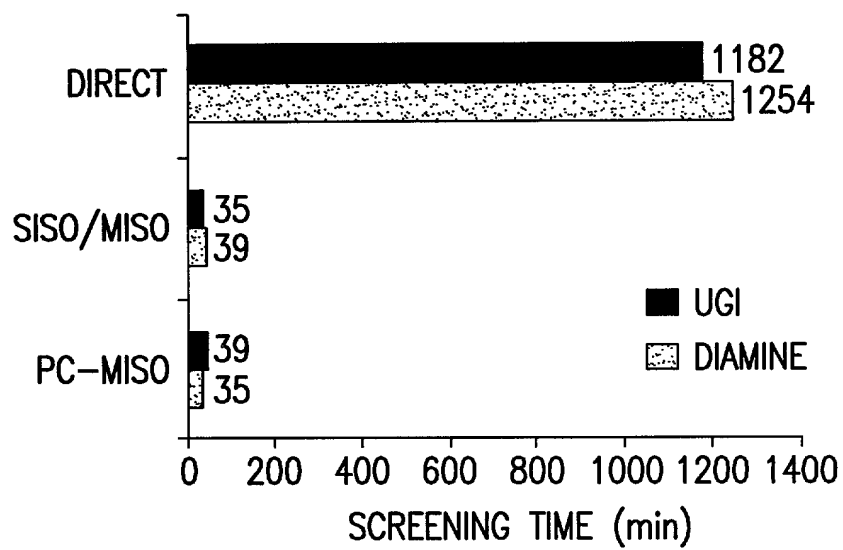
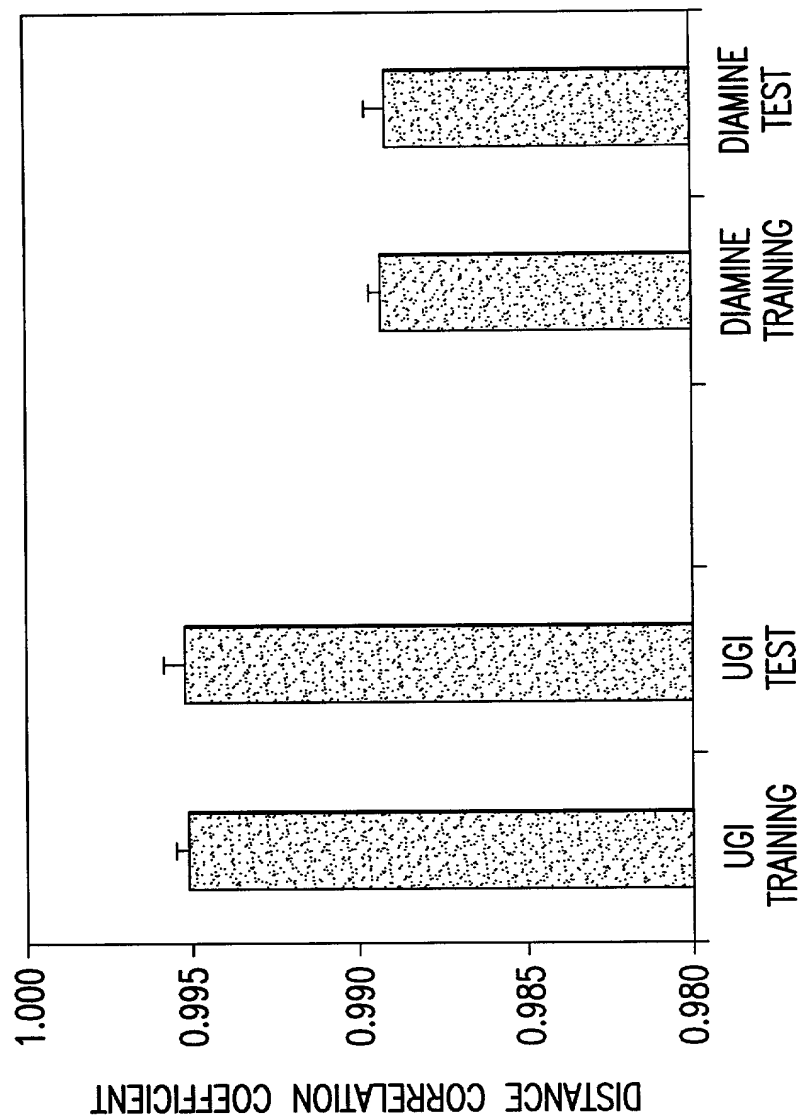


FIG.6



Appl. No. 09/934,084; Group Art Unit: 2857
 Dkt. No. 1503.1070003; Batch No.: N/A
 Inventor(s): Lobanov et al.; Tel: 202/371-2600
 Title: Method, System, and Computer Program Product for
 Determining Properties of Combinatorial Library Products...

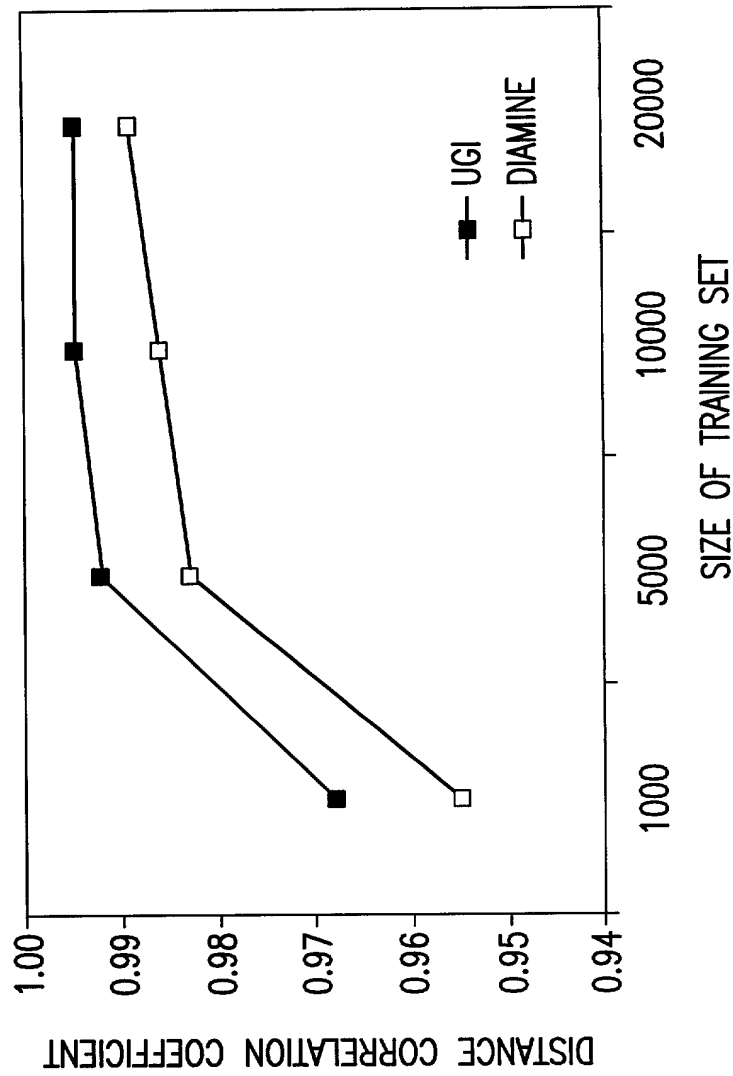


FIG.8

Appl. No. 09/934,084; Group Art Unit: 2857
 Dkt. No. 1503.1070003; Batch No.: N/A
 Inventor(s): Lobanov et al.; Tel: 202/371-2600
 Title: Method, System, and Computer Program Product for
 Determining Properties of Combinatorial Library Products...

| INDEX | DESCRIPTOR | SISO TRAINING R ² | SISO TEST R ² | MISO TRAINING R ² | MISO TEST R ² |
|-------|--------------------|------------------------------------|--------------------------------|------------------------------------|--------------------------------|
| 1 | NO. ATOMS | 0.996 | 0.997 | | |
| 2 | NO. BONDS | 0.995 | 0.996 | | |
| 3 | NO. ELEMENTS | 0.603 | 0.614 | 0.822 | 0.823 |
| 4 | MOLECULAR WEIGHT | 0.996 | 0.997 | | |
| 5 | CHI 0 | 0.996 | 0.997 | | |
| 6 | CHI PATH 1 | 0.996 | 0.997 | | |
| 7 | CHI PATH 2 | 0.994 | 0.995 | | |
| 8 | CHI PATH 3 | 0.971 | 0.973 | | |
| 9 | CHI PATH 4 | 0.974 | 0.976 | | |
| 10 | CHI PATH 5 | 0.956 | 0.957 | | |
| 11 | CHI PATH 6 | 0.909 | 0.910 | | |
| 12 | CHI PATH 7 | 0.837 | 0.843 | 0.943 | 0.942 |
| 13 | CHI PATH 8 | 0.666 | 0.673 | 0.938 | 0.934 |
| 14 | CHI PATH 9 | 0.563 | 0.554 | 0.939 | 0.936 |
| 15 | CHI PATH 10 | 0.447 | 0.457 | 0.950 | 0.950 |
| 16 | CHI CLUSTER 3 | 0.988 | 0.987 | | |
| 17 | CHI CLUSTER 4 | 0.993 | 0.993 | | |
| 18 | CHI PATH/CLUSTER 4 | 0.978 | 0.980 | | |
| 19 | VAL CHI 0 | 0.996 | 0.997 | | |
| 20 | VAL CHI PATH 1 | 0.997 | 0.998 | | |
| 21 | VAL CHI PATH 2 | 0.996 | 0.996 | | |
| 22 | VAL CHI PATH 3 | 0.993 | 0.994 | | |
| 23 | VAL CHI PATH 4 | 0.981 | 0.982 | | |
| 24 | VAL CHI PATH 5 | 0.952 | 0.951 | | |
| 25 | VAL CHI PATH 6 | 0.907 | 0.905 | | |

FIG. 9A

Appl. No. 09/934,084; Group Art Unit: 2857
 Dkt. No. 1503.1070003; Batch No.: N/A
 Inventor(s): Lobanov et al.; Tel: 202/371-2600
 Title: Method, System, and Computer Program Product for
 Determining Properties of Combinatorial Library Products...

| INDEX | DESCRIPTOR | SISO TRAINING R ² | SISO TEST R ² | MISO TRAINING R ² | MISO TEST R ² |
|-------|------------------------|------------------------------------|--------------------------------|------------------------------------|--------------------------------|
| 26 | VAL CHI PATH 7 | 0.773 | 0.775 | 0.901 | 0.905 |
| 27 | VAL CHI PATH 8 | 0.619 | 0.621 | 0.890 | 0.889 |
| 28 | VAL CHI PATH 9 | 0.349 | 0.328 | 0.910 | 0.910 |
| 29 | VAL CHI PATH 10 | 0.222 | 0.201 | 0.921 | 0.920 |
| 30 | VAL CHI CLUSTER 3 | 0.994 | 0.994 | | |
| 31 | VAL CHI CLUSTER 4 | 0.993 | 0.993 | | |
| 32 | VAL CHI PATH/CLUSTER 4 | 0.988 | 0.989 | | |
| 33 | CHI CHAIN 3 | 1.000 | 1.000 | | |
| 34 | CHI CHAIN 4 | 1.000 | 1.000 | | |
| 35 | CHI CHAIN 5 | 0.979 | 0.978 | | |
| 36 | CHI CHAIN 6 | 0.995 | 0.995 | | |
| 37 | CHI CHAIN 7 | 0.999 | 0.999 | | |
| 38 | CHI CHAIN 8 | 1.000 | 1.000 | | |
| 39 | CHI CHAIN 9 | 0.999 | 0.999 | | |
| 40 | CHI CHAIN 10 | 0.999 | 0.998 | | |
| 41 | VAL CHI CHAIN 3 | 1.000 | 1.000 | | |
| 42 | VAL CHI CHAIN 4 | 1.000 | 1.000 | | |
| 43 | VAL CHI CHAIN 5 | 0.994 | 0.996 | | |
| 44 | VAL CHI CHAIN 6 | 0.994 | 0.995 | | |
| 45 | VAL CHI CHAIN 7 | 0.998 | 0.998 | | |
| 46 | VAL CHI CHAIN 8 | 1.000 | 1.000 | | |
| 47 | VAL CHI CHAIN 9 | 0.997 | 0.998 | | |
| 48 | VAL CHI CHAIN 10 | 0.986 | 0.980 | | |
| 49 | SUBGRAPH COUNT PATH 2 | 0.996 | 0.997 | | |
| 50 | SUBGRAPH COUNT PATH 3 | 0.990 | 0.990 | | |

FIG. 9B

| INDEX | DESCRIPTOR | SISO TRAINING R ² | SISO TEST R ² | MISO TRAINING R ² | MISO TEST R ² |
|-------|-------------------------------|------------------------------------|--------------------------------|------------------------------------|--------------------------------|
| 51 | SUBGRAPH COUNT PATH 4 | 0.957 | 0.960 | | |
| 52 | SUBGRAPH COUNT PATH 5 | 0.914 | 0.918 | | |
| 53 | SUBGRAPH COUNT PATH 6 | 0.837 | 0.844 | 0.909 | 0.905 |
| 54 | SUBGRAPH COUNT PATH 7 | 0.752 | 0.770 | 0.892 | 0.887 |
| 55 | SUBGRAPH COUNT PATH 8 | 0.582 | 0.599 | 0.907 | 0.906 |
| 56 | SUBGRAPH COUNT PATH 9 | 0.446 | 0.448 | 0.933 | 0.932 |
| 57 | SUBGRAPH COUNT PATH 10 | 0.366 | 0.383 | 0.947 | 0.945 |
| 58 | SUBGRAPH COUNT CLUSTER 3 | 0.994 | 0.995 | | |
| 59 | SUBGRAPH COUNT CLUSTER 4 | 0.991 | 0.991 | | |
| 60 | SUBGRAPH COUNT PATH/CLUSTER 4 | 0.980 | 0.980 | | |
| 61 | SUBGRAPH COUNT RING 3 | 1.000 | 1.000 | | |
| 62 | SUBGRAPH COUNT RING 4 | 1.000 | 1.000 | | |
| 63 | SUBGRAPH COUNT RING 5 | 0.995 | 0.995 | | |
| 64 | SUBGRAPH COUNT RING 6 | 0.994 | 0.995 | | |
| 65 | SUBGRAPH COUNT RING 7 | 1.000 | 1.000 | | |
| 66 | SUBGRAPH COUNT RING 8 | 1.000 | 1.000 | | |
| 67 | SUBGRAPH COUNT RING 9 | 1.000 | 1.000 | | |
| 68 | SUBGRAPH COUNT RING 10 | 0.999 | 0.999 | | |
| 69 | KAPPA 0 | 0.980 | 0.980 | | |
| 70 | KAPPA 1 | 0.991 | 0.992 | | |
| 71 | KAPPA 2 | 0.907 | 0.908 | | |
| 72 | KAPPA 3 | 0.709 | 0.710 | 0.806 | 0.799 |
| 73 | KAPPA ALPHA 1 | 0.987 | 0.987 | | |
| 74 | KAPPA ALPHA 2 | 0.895 | 0.897 | 0.960 | 0.955 |
| 75 | KAPPA ALPHA 3 | 0.685 | 0.686 | 0.774 | 0.770 |

FIG. 9C

| INDEX | DESCRIPTOR | SISO TRAINING R ² | SISO TEST R ² | MISO TRAINING R ² | MISO TEST R ² |
|-------|--------------------------------------|------------------------------------|--------------------------------|------------------------------------|--------------------------------|
| 76 | WIENER PATH NO. | 0.967 | 0.965 | | |
| 77 | TOTAL WIENER PATH NO. | 0.903 | 0.892 | | |
| 78 | SHANNON INDEX | 0.911 | 0.911 | | |
| 79 | TOTAL NO. OF PATHS | 0.939 | 0.932 | | |
| 80 | BONCHEV-TRINAJSTIĆ IdW INDEX | 0.958 | 0.955 | | |
| 81 | BONCHEV-TRINAJSTIĆ MEAN IdW INDEX | 0.972 | 0.972 | | |
| 82 | BONCHEV-TRINAJSTIĆ IdC INDEX | 0.979 | 0.978 | | |
| 83 | BONCHEV-TRINAJSTIĆ MEAN IdC INDEX | 0.793 | 0.773 | 0.707 | 0.759 |
| 84 | WIENER PARITY NO. | 0.988 | 0.989 | | |
| 85 | PLATT F NO. | 0.996 | 0.997 | | |
| 86 | DELTA PARTITION 1 | 0.996 | 0.996 | | |
| 87 | DELTA PARTITION 2 | 0.992 | 0.992 | | |
| 88 | DELTA PARTITION 3 | 0.997 | 0.997 | | |
| 89 | DELTA PARTITION 4 | 0.995 | 0.996 | | |
| 90 | DELTA PARTITION 5 | 1.000 | 1.000 | | |
| 91 | DELTA PARTITION 6 | 1.000 | 1.000 | | |
| 92 | NO. H | 0.996 | 0.997 | | |
| 93 | NO. B | 1.000 | 1.000 | | |
| 94 | No. C | 0.997 | 0.998 | | |
| 95 | No. N | 0.995 | 0.995 | | |
| 96 | No. O | 0.994 | 0.993 | | |
| 97 | No. F | 0.996 | 0.996 | | |
| 98 | No. Si | 1.000 | 1.000 | | |
| 99 | No. P | 0.999 | 0.999 | | |

FIG. 9D

Appl. No. 09/934,084; Group Art Unit: 2857
 Dkt. No. 1503.1070003; Batch No.: N/A
 Inventor(s): Lobanov et al.; Tel: 202/371-2600
 Title: Method, System, and Computer Program Product for
 Determining Properties of Combinatorial Library Products...

| INDEX | DESCRIPTOR | SISO TRAINING R ² | SISO TEST R ² | MISO TRAINING R ² | MISO TEST R ² |
|-------|----------------------------|------------------------------------|--------------------------------|------------------------------------|--------------------------------|
| 100 | No. S | 0.997 | 0.999 | | |
| 101 | No. Cl | 0.997 | 0.997 | | |
| 102 | No. Ge | 1.000 | 1.000 | | |
| 103 | No. As | 1.000 | 1.000 | | |
| 104 | No. Se | 1.000 | 1.000 | | |
| 105 | No. Br | 1.000 | 1.000 | | |
| 106 | No. I | 1.000 | 1.000 | | |
| 107 | NO. HALOGENS | 0.997 | 0.998 | | |
| 108 | TOTAL TOPOLOGICAL STATE 1 | 0.924 | 0.918 | | |
| 109 | TOTAL TOPOLOGICAL STATE 2 | 0.947 | 0.945 | | |
| 110 | TOTAL TOPOLOGICAL STATE 3 | 0.904 | 0.888 | | |
| 111 | TOTAL TOPOLOGICAL STATE 4 | 0.956 | 0.956 | | |
| 112 | TOTAL TOPOLOGICAL STATE 5 | 0.852 | 0.826 | 0.915 | 0.907 |
| 113 | TOTAL TOPOLOGICAL STATE 6 | 0.980 | 0.980 | | |
| 114 | TOTAL TOPOLOGICAL STATE 7 | 0.832 | 0.790 | 0.914 | 0.889 |
| 115 | TOTAL TOPOLOGICAL STATE 8 | 0.988 | 0.988 | | |
| 116 | TOTAL TOPOLOGICAL STATE 9 | 0.913 | 0.909 | | |
| 117 | TOTAL TOPOLOGICAL STATE 10 | 0.922 | 0.918 | | |

FIG. 9E

| LEAD | RANDOM | DIRECT | SISO/MISO | SISO/MISO | PC-MISO | PC-MISO |
|------|------------|------------|------------|-----------|------------|----------|
| | SIMILARITY | SIMILARITY | SIMILARITY | IDENTITY | SIMILARITY | IDENTITY |
| 1 | 1.754 | 0.480 | 0.501 | 69% | 0.486 | 86% |
| 2 | 1.158 | 0.238 | 0.279 | 56% | 0.244 | 83% |
| 3 | 1.664 | 0.655 | 0.680 | 64% | 0.660 | 84% |
| 4 | 1.291 | 0.179 | 0.213 | 60% | 0.186 | 76% |
| 5 | 1.763 | 0.327 | 0.335 | 82% | 0.334 | 83% |
| 6 | 1.196 | 0.201 | 0.224 | 58% | 0.209 | 75% |
| 7 | 1.294 | 0.274 | 0.291 | 72% | 0.283 | 77% |
| 8 | 1.385 | 0.268 | 0.288 | 73% | 0.275 | 84% |
| 9 | 1.694 | 0.464 | 0.481 | 74% | 0.470 | 86% |
| 10 | 1.613 | 0.460 | 0.470 | 79% | 0.464 | 87% |

FIG.10

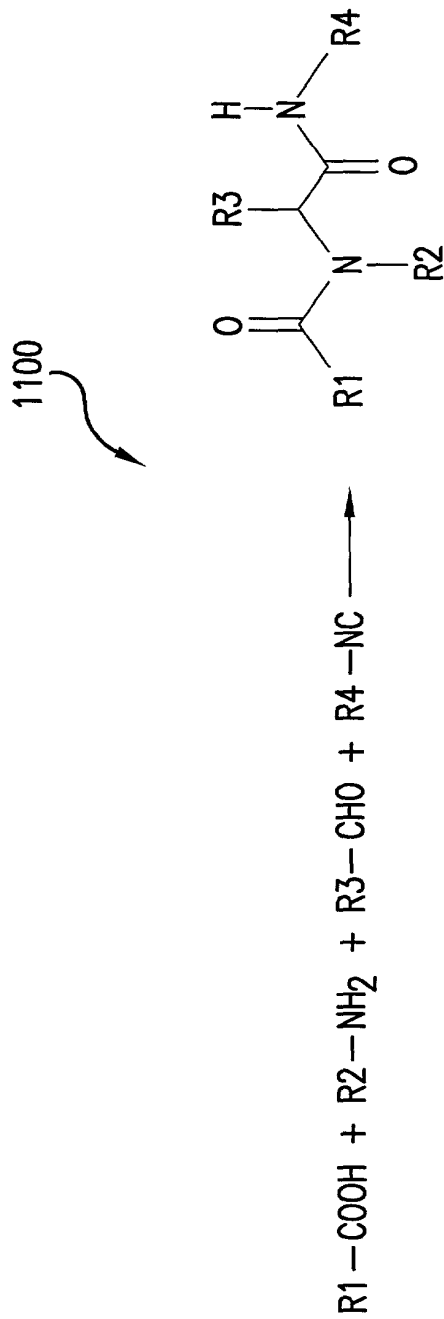


FIG. 11

Appl. No. 09/934,084; Group Art Unit: 2857
 Dkt. No. 1503.1070003; Batch No.: N/A
 Inventor(s): Lobanov et al.; Tel: 202/371-2600
 Title: Method, System, and Computer Program Product for
 Determining Properties of Combinatorial Library Products...

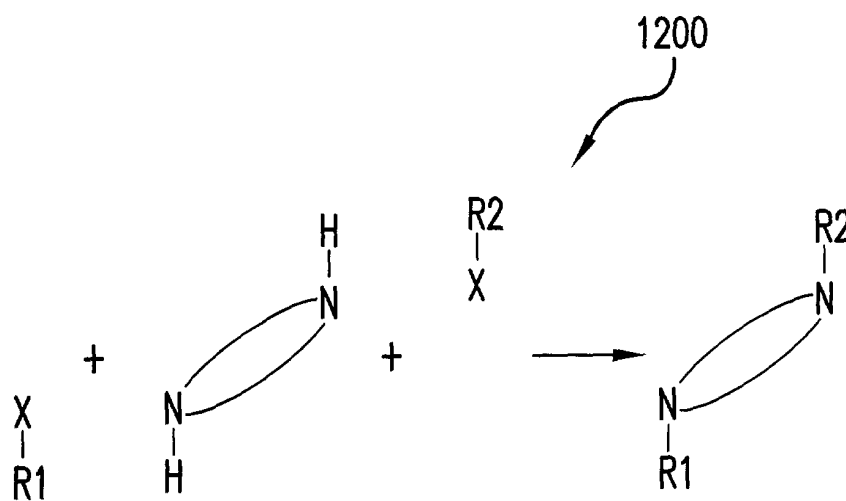


FIG. 12

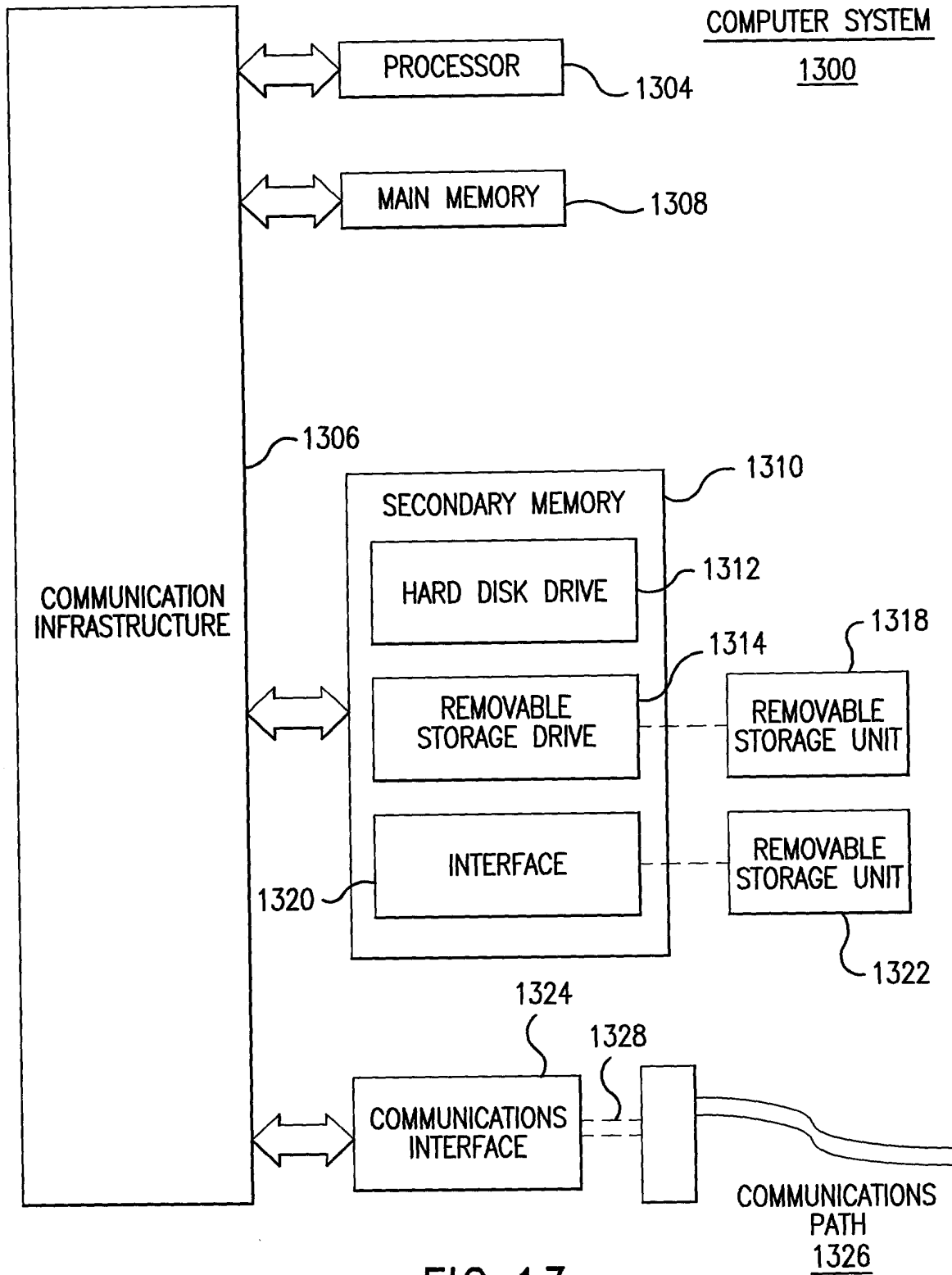


FIG. 13